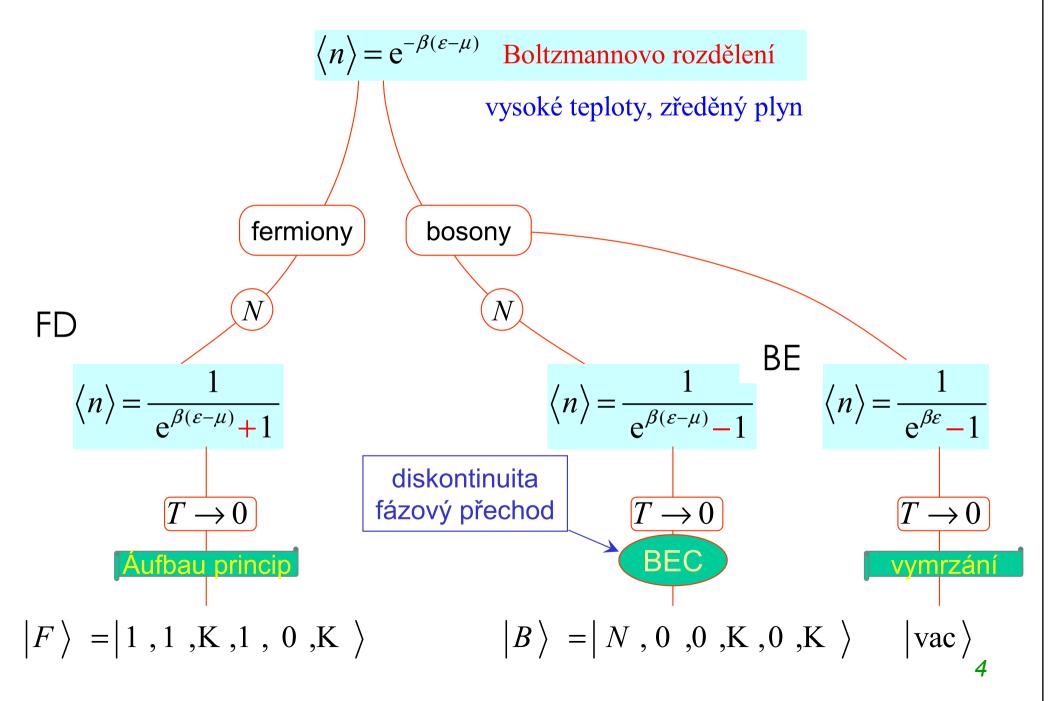
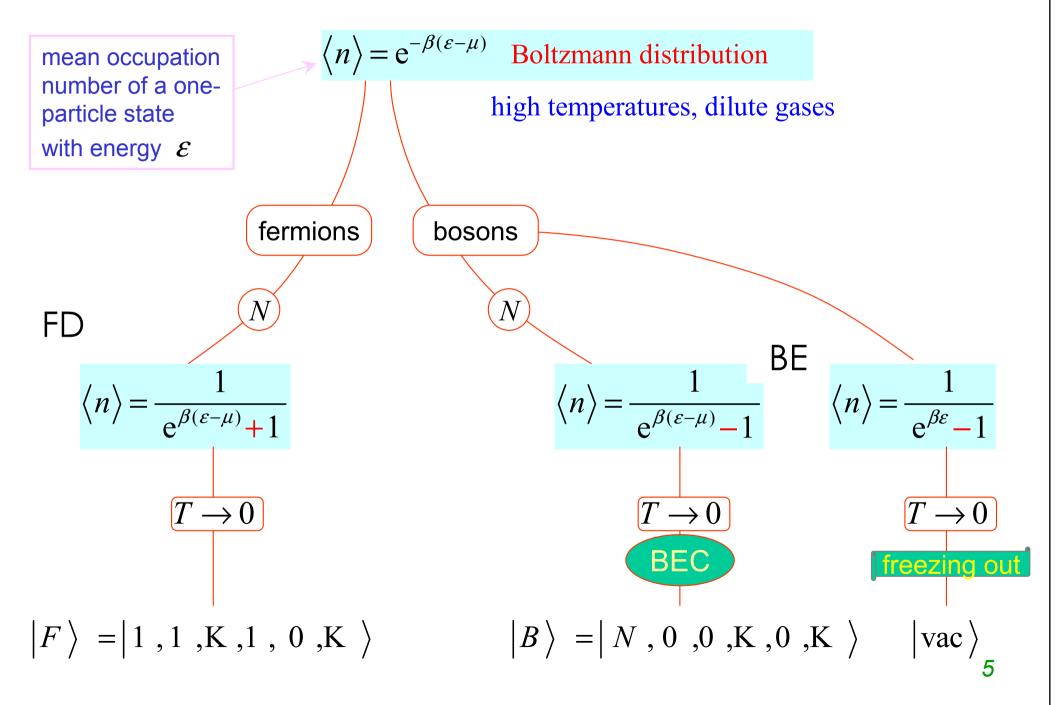
# Cold atoms

Lecture 2. 10. October 2007 BEC for independent particles Two basic models: BEC in an ideal gas vs. in a trapped atomic cloud Problems with thermodynamic limit BEC for independent particles

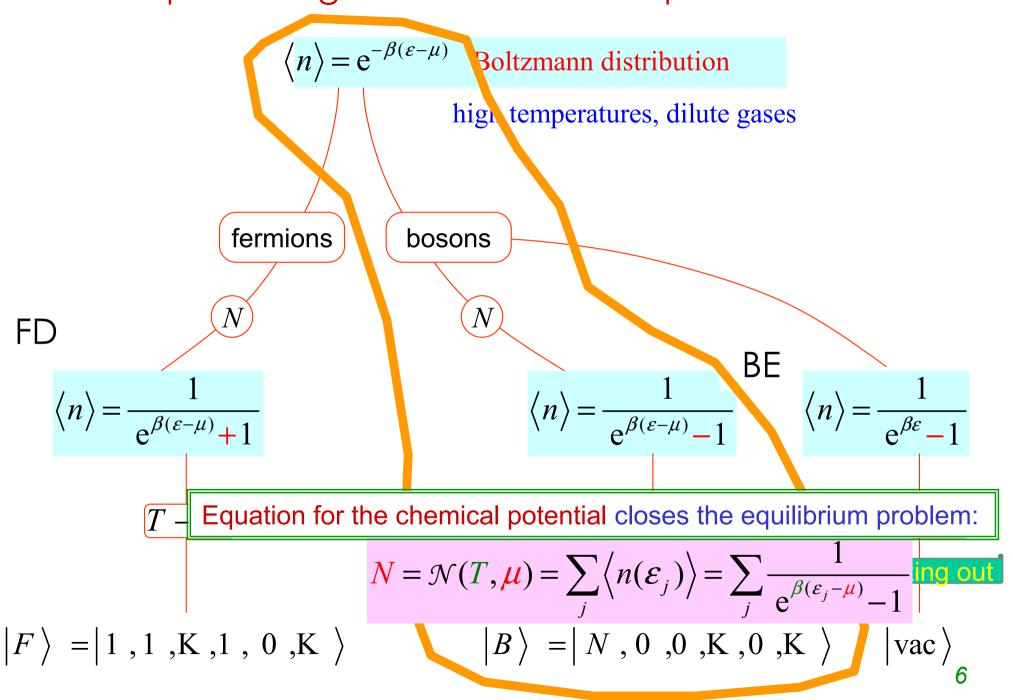
### LAST TIME Ideální kvantové plyny



#### Ideal quantum gases at a finite temperature



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volume V, particle number N, density n=N/V, temperature T.

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$$N \approx V \int_{0}^{\infty} \mathrm{d} \varepsilon \frac{1}{\mathrm{e}^{\beta(\varepsilon - \mu)} - 1} \mathcal{D}(\varepsilon) \equiv \mathcal{N}(T, \mu)$$

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It holds

$$\mathscr{N}(T,\mu<0)<\mathscr{N}(T,0)<\infty$$

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For each temperature, we get a critical number of atoms the gas can accommodate. Where will go the rest? To the condensate 12

### Condensate concentration

#### The integral is doable:

 $\mathcal{N}(T,0) = V \int_{0}^{\infty} \mathrm{d}\varepsilon \frac{1}{\mathrm{e}^{\beta\varepsilon} - 1} \mathcal{D}(\varepsilon)$ 

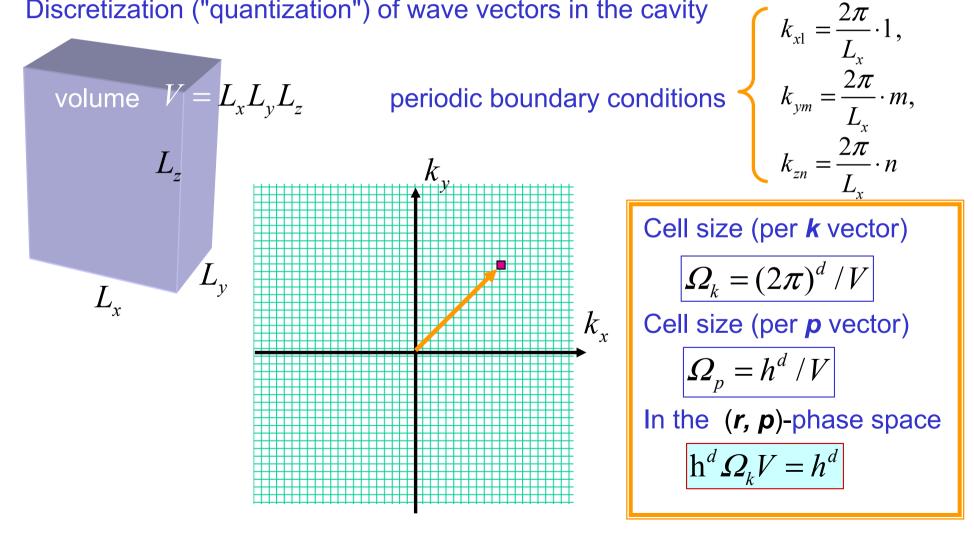
use the general formula

#### Plane waves in a cavity

Plane wave in classical terms and its quantum transcription

$$X = X_0 e^{-i(\omega t - \mathbf{k} \cdot \mathbf{r})}, \quad \omega = \omega(k), \quad \lambda = 2\pi / k$$
  
 $\varepsilon = h\omega, \quad \mathbf{p} = h\mathbf{k}, \quad \varepsilon = \varepsilon(p), \quad \lambda = h / p \text{ de Broglie wavelength}$ 

Discretization ("quantization") of wave vectors in the cavity



### Density of states

**IDOS** Integrated Density Of States:

How many states have energy less than  $\boldsymbol{\varepsilon}$ Invert the dispersion law

$$\mathcal{E}(p) \quad \Box \quad p(\mathcal{E})$$

Find the volume of the *d*-sphere in the *p*-space

$$\mathcal{Q}_d(p) = C_d \cdot p^d$$

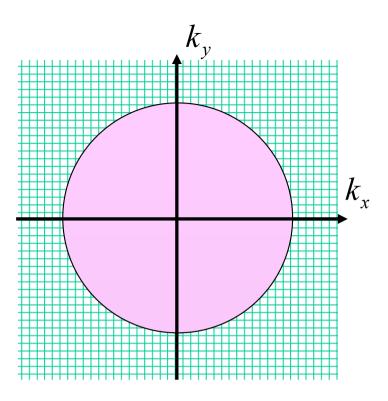
Divide by the volume of the cell

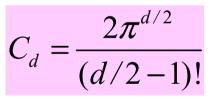
$$\Gamma(\varepsilon) = \Omega_d(p(\varepsilon)) / \Omega_p = V \cdot \Omega_d(p(\varepsilon)) / h^d$$

DOS Density Of States:

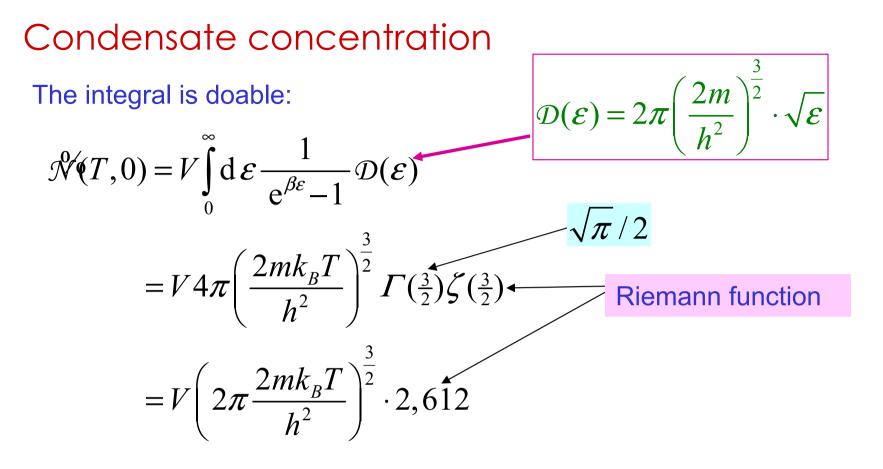
How many states are around  $\mathcal{E}$  per unit energy per unit volume

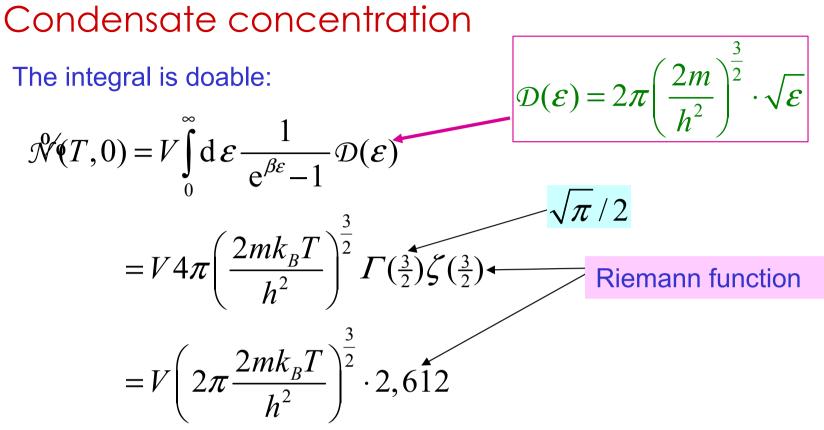
$$\begin{aligned} \mathcal{D}(\varepsilon) &= \frac{1}{V} \frac{\mathrm{d}}{\mathrm{d}\varepsilon} \Gamma(\varepsilon) \\ &= \frac{\mathrm{d}}{\mathrm{d}\varepsilon} \Omega_d (p(\varepsilon)/h)^d = dC_d h^{-1} \cdot (p(\varepsilon)/h)^{d-1} \frac{\mathrm{d} p(\varepsilon)}{\mathrm{d}\varepsilon} \end{aligned}$$







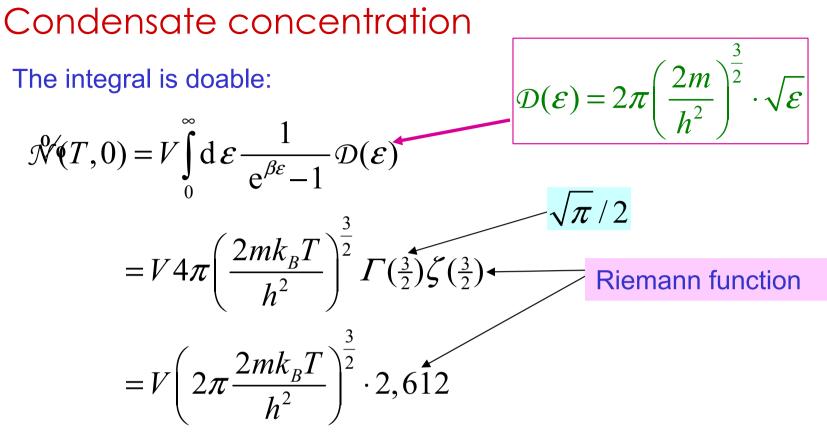




CRITICAL TEMPERATURE

the lowest temperature at which all atoms are still accomodated in the gas:

$$\mathcal{N}(T_c,0) = N$$



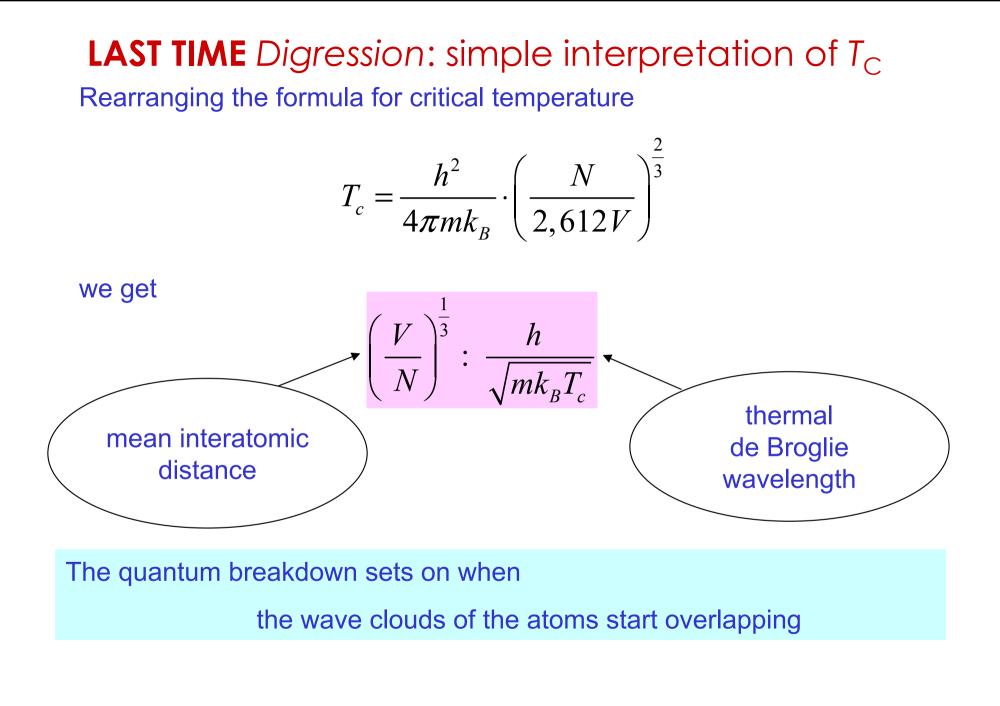
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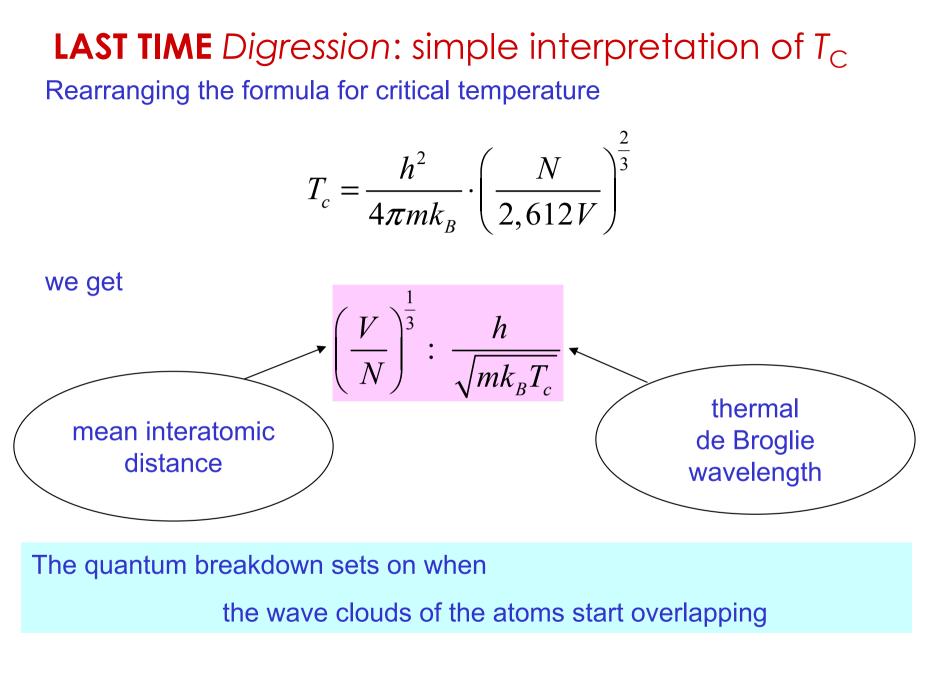
the lowest temperature at which all atoms are still accomodated in the gas:

$$\mathcal{N}(T_c, 0) = N$$
 atomic mass  
$$T_c = \frac{h^2}{4\pi m k_B} \cdot \left(\frac{N}{2,612V}\right)^{\frac{2}{3}} = 0,52725 \frac{h^2}{4\pi u k_B} \cdot \frac{n^{\frac{2}{3}}}{M} = 1,6061 \times 10^{-18} \cdot \frac{n^{\frac{2}{3}}}{M}$$

## From a gas to an inhomogeneous system

Physical interpretation of BEC Where are the condensate Bosons?





NICE, BUT TOO SPECIFIC FOR A GAS

#### **LAST TIME** What is the nature of BEC?

With lowering the temperature, the atoms of the gas lose their energy and drain down to the lowest energy states. There is less and less of these:

 $\mathcal{N}(E < k_B T) = \operatorname{const} \times T^{3/2}$ 

A given amount N of the atoms becomes too large starting from a critical temperature.

Their excess precipitates to the lowest level, which becomes *macroscopically occupied,* i.e., it holds a finite fraction of all atoms.

This is the BE condensate.

At the zero temperature, all atoms are in the condensate.

Einstein was the first to realize that and to make an exact calculation of the integrals involved.

$$\mathcal{N}_{G}^{0}(T) = V \times 4\pi \left(\frac{2mk_{B}T}{h^{2}}\right)^{\frac{3}{2}} \Gamma(\frac{3}{2})\zeta(\frac{3}{2}) \equiv BT^{\frac{3}{2}}$$

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Where are the condensate atoms?

ANSWER: On the lowest one-particle energy level

For understanding, return to the discrete levels.

$$N = \mathcal{N}(T, \mu) = \sum_{j} \left\langle n(\varepsilon_{j}) \right\rangle = \sum_{j} \frac{1}{e^{\beta(\varepsilon_{j} - \mu)} - 1}$$

There is a sequence of energies

$$\mu < \varepsilon_0 = \varepsilon(0) = 0 < \varepsilon_1 < \varepsilon_2 L$$

For very low temperatures,  $\beta(\varepsilon_1 - \varepsilon_0)$ ? 1

all atoms are on the lowest level, so that

 $n_{0} = N - O(e^{-\beta(\varepsilon_{1} - \varepsilon_{0})}) \quad \text{all atoms are in the condensate}$   $N \approx \frac{1}{e^{\beta(\varepsilon_{0} - \mu)} - 1} \quad \text{connecting equation}$   $\mu \approx \varepsilon_{0} - \frac{k_{B}T}{N} \quad \text{chemical potential is zero on the gross energy scale}$ 

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#### Where are the condensate atoms? Continuation

ANSWER: On the lowest one-particle energy level

For temperatures below  $T_C$ 

all condensate atoms are on the lowest level, so that

 $n_{0} = N_{BE}$  all condensate atoms remain on the lowest level  $N_{BE} \approx \frac{1}{e^{\beta(\varepsilon_{0}-\mu)}-1}$  connecting equation  $\mu \approx \varepsilon_{0} - \frac{k_{B}T}{N_{BE}}$  chemical potential keeps zero on the gross energy scale

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question ... what happens with the occupancy of the next level now? Estimate:  $2^{2}$ 

$$\boldsymbol{\mathcal{E}}_1 - \boldsymbol{\mathcal{E}}_0 : \left( h^2 / m \right) \cdot V^{-3}$$

$$n_0 = \frac{k_B T}{\varepsilon_0 - \mu} = O(V), \quad n_1 = \frac{k_B T}{\varepsilon_1 - \mu} = O(V^{\frac{2}{3}}) \quad \dots \text{ much slower growth}$$

### Where are the condensate atoms? Summary

ANSWER: On the lowest one-particle energy level

The final balance equation for  $T < T_C$  is

$$N = \mathcal{N}(T, \mu) = \frac{1}{e^{\beta(\varepsilon_0 - \mu)} - 1} + V \int_0^\infty d\varepsilon \frac{1}{e^{\beta(\varepsilon - \mu)} - 1} \mathcal{D}(\varepsilon)$$

LESSON:

be slow with making the thermodynamic limit (or any other limits)

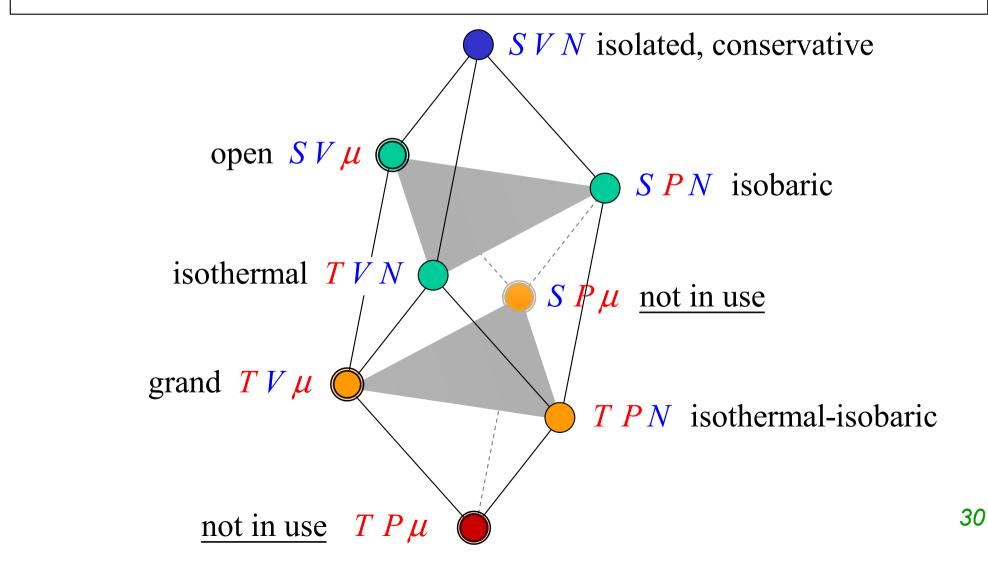
## Thermodynamics of BEC

Capsule on thermodynamics Grand canonical ensemble Thermodynamic functions of an ideal gas BEC in an ideal gas Homogeneous one component phase: boundary conditions (environment) and state variables

SVN additive variables, have densities s = S/V n = N/V "extensive" b b b

 $T P \mu$  dual variables, intensities

"intensive"

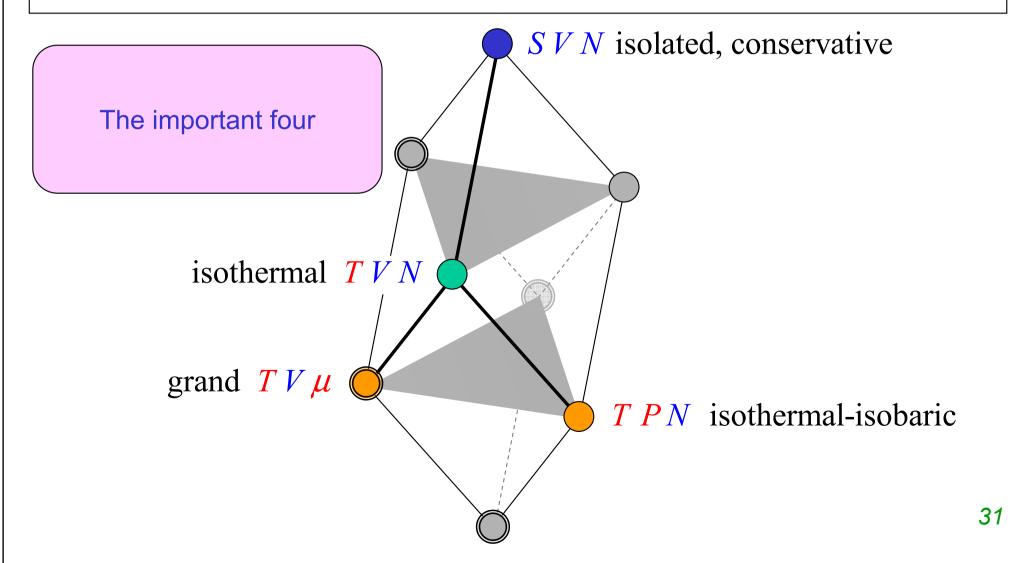


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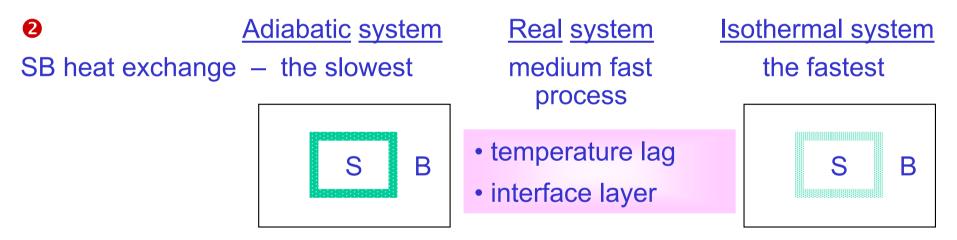
### Digression: which environment to choose?

#### THE ENVIRONMENT IN THE THEORY SHOULD CORRESPOND TO THE EXPERIMENTAL CONDITIONS

... a truism difficult to satisfy

• For large systems, this is not so sensitive for two reasons

- System serves as a thermal bath or particle reservoir all by itself
- Relative fluctuations (distinguishing mark) are negligible



Atoms in a trap: ideal model ... isolated. In fact: unceasing energy exchange (laser cooling). A small number of atoms may be kept (one to, say, 40). With 10<sup>7</sup>, they form a bath already. Besides, they are cooled by evaporation and they form an open (albeit non-equilibrium) system.

Some people, notably *Leggett*, insist on using clouds with a fixed number of atoms. This changes the physics of BEC substantially!
 32

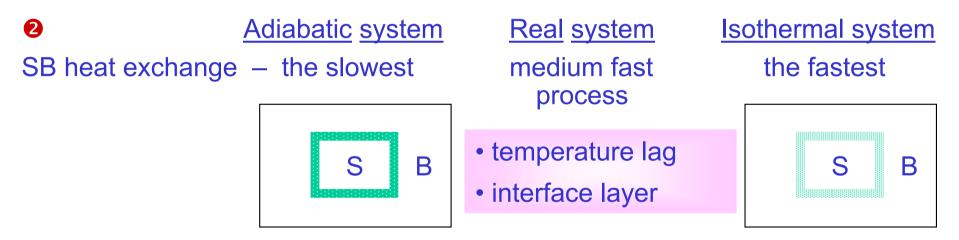
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## Grand canonical ensemble

Definition following Gibbs General treatment for independent particles Thermodynamic functions of an ideal gas

#### Grand canonical ensemble - definition

<u>Grand canonical ensemble</u> admits both energy and particle number exchange between the system and its environment.

The statistical operator (many body density matrix)  $\hat{\rho}$  acts in the Fock space

External variables are  $T, V, \mu$ . They are specified by the conditions

$$\langle \hat{H} \rangle \equiv \operatorname{Tr} \hat{\rho} \hat{H} = U$$
  $V = \operatorname{sharp}$   $\langle \hat{N} \rangle \equiv \operatorname{Tr} \hat{\rho} \hat{N} = N$   
 $S = -k_{\mathrm{B}} \cdot \operatorname{Tr} \hat{\rho} \ln \hat{\rho} = \max$ 

Grand canonical statistical operator has the Gibbs' form

$$\hat{\rho} = Z^{-1} e^{-\beta(\hat{H} - \mu\hat{N})}$$

$$Z(\beta, \mu, V) = \operatorname{Tr} e^{-\beta(\hat{H} - \mu\hat{N})} \equiv e^{-\beta\Omega(\beta, \mu, V)} \text{ statistical sum}$$

$$\Omega(\beta, \mu, V) = -k_{\mathrm{B}}T \ln Z(\beta, \mu, V) \text{ grand canonical potential}$$

#### Grand canonical ensemble – general definition

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volume ... for an extended homogeneous system

*V* ... generic for generalized coordinates of external fields whose change is connected with the mechanical work done by the system

### Fluctuations I. – global quantities

Fluctuations of the total number of particles around the mean value

First derivative of the grand potential

$$\frac{\partial \Omega}{\partial \mu} = \frac{\partial}{\partial \mu} \left( -k_{\rm B} T \ln Z \right) = -k_{\rm B} T \frac{\partial}{\partial \mu} \ln \operatorname{Tr} e^{-\beta(\hat{H} - \mu\hat{N})} = -\frac{\operatorname{Tr} \hat{N} e^{-\beta(\hat{H} - \mu\hat{N})}}{\operatorname{Tr} e^{-\beta(\hat{H} - \mu\hat{N})}} = -\left\langle \hat{N} \right\rangle$$

Second derivative of the grand potential

$$\frac{\partial^2 \Omega}{\partial \mu^2} = -\frac{\partial}{\partial \mu} \left\langle \hat{N} \right\rangle = -\frac{\partial}{\partial \mu} \frac{\operatorname{Tr} \hat{N} e^{-\beta(\hat{H} - \mu\hat{N})}}{\operatorname{Tr} e^{-\beta(\hat{H} - \mu\hat{N})}} = -\frac{\operatorname{Tr} \hat{N}^2 e^{-\beta(\hat{H} - \mu\hat{N})}}{\operatorname{Tr} e^{-\beta(\hat{H} - \mu\hat{N})}} + \frac{(\operatorname{Tr} \hat{N} e^{-\beta(\hat{H} - \mu\hat{N})})^2}{(\operatorname{Tr} e^{-\beta(\hat{H} - \mu\hat{N})})^2} = -\left\langle \hat{N}^2 \right\rangle + \left\langle \hat{N} \right\rangle^2$$

Final estimate for the relative fluctuation

$$\frac{\left\langle \hat{N}^{2} \right\rangle - \left\langle \hat{N} \right\rangle^{2}}{\left\langle \hat{N} \right\rangle^{2}} = \frac{\frac{\partial}{\partial \mu} \left\langle \hat{N} \right\rangle}{\left\langle \hat{N} \right\rangle^{2}} = O\left(\left\langle \hat{N} \right\rangle^{-1}\right)$$

## Grand canonical statistical sum for independent bosons

$$\begin{aligned} & |Z(\beta,\mu,V) = \mathrm{Tr} \, \mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}| = \mathrm{e}^{-\beta\Omega(\beta,\mu,V)} \text{ statistical sum} \\ &= \sum_{1} \mathrm{e}^{-\beta(E_{1}-\mu N_{1})} \qquad \mathrm{IK} \text{ eigenstate label } 1 \equiv \{n_{\alpha}\} \text{ with } \sum_{\alpha} n_{\alpha} = N_{1} \\ &= \sum_{n_{\alpha}} \mathrm{e}^{-\beta\sum_{\alpha}(\varepsilon_{\alpha}-\mu)n_{\alpha}} = \sum_{\{n_{\alpha}\}} \prod_{\alpha} \left( \mathrm{e}^{-\beta(\varepsilon_{\alpha}-\mu)} \right)^{n_{\alpha}} \text{ up to here trivial} \end{aligned}$$

$$\begin{aligned} &= \mathrm{TRICK!!} = \prod_{\alpha} \sum_{n_{\alpha}} \left( \mathrm{e}^{-\beta(\varepsilon_{\alpha}-\mu)} \right)^{n_{\alpha}} = \prod_{\alpha} \frac{1}{1-\mathrm{e}^{-\beta(\varepsilon_{\alpha}-\mu)}} \\ &= \lim_{\alpha} \frac{1}{1-\mathrm{e}^{-\beta(\varepsilon_{\alpha}-\mu)}} = \prod_{\alpha} \frac{1}{1-\mathrm{z} \, \mathrm{e}^{-\beta\varepsilon_{\alpha}}} \end{aligned}$$

$$\begin{aligned} &= k_{\mathrm{B}}T \sum_{\alpha} \ln\left(1-\mathrm{e}^{-\beta(\varepsilon_{\alpha}-\mu)}\right) \\ &= +k_{\mathrm{B}}T \sum_{\alpha} \ln\left(1-\mathrm{z} \, \mathrm{e}^{-\beta\varepsilon_{\alpha}}\right) \end{aligned}$$

## Grand canonical statistical sum for independent bosons

Recall  

$$\begin{aligned} |Z(\beta,\mu,V)| &= \operatorname{Tr} e^{-\beta(\hat{H}-\mu\hat{N})} = e^{-\beta\Omega(\beta,\mu,V)} \text{ statistical sum} \\ &= \sum_{l} e^{-\beta(E_{l}-\mu N_{l})} \quad lK \text{ eigenstate label } 1 = \{n_{\alpha}\} \text{ with } \sum_{\alpha} n_{\alpha} = N_{l} \\ &= \sum_{l} e^{-\beta\sum_{\alpha}(\varepsilon_{\alpha}-\mu)n_{\alpha}} = \sum_{\{n_{\alpha}\}} \prod_{\alpha} \left( e^{-\beta(\varepsilon_{\alpha}-\mu)} \right)^{n_{\alpha}} \text{ up to here trivial} \end{aligned}$$

$$\begin{aligned} \overline{\operatorname{TRICK!!}} &= \prod_{\alpha} \sum_{n_{\alpha}} \left( e^{-\beta(\varepsilon_{\alpha}-\mu)} \right)^{n_{\alpha}} = \prod_{\alpha} \frac{1}{1-e^{-\beta(\varepsilon_{\alpha}-\mu)}} \\ e^{\beta\mu} \equiv z \quad \operatorname{activity}_{fugacity} \end{aligned}$$

$$\begin{aligned} Z(\beta,\mu,V) &= \prod_{\alpha} \frac{1}{1-e^{-\beta(\varepsilon_{\alpha}-\mu)}} \equiv \prod_{\alpha} \frac{1}{1-z e^{-\beta\varepsilon_{\alpha}}} \end{aligned}$$

$$\begin{aligned} \mathrm{symbolic \ control\ parameter}_{riminite^{\alpha}\ gas} \\ &= +k_{\mathrm{B}}T \sum_{\alpha} \ln\left(1-z e^{-\beta\varepsilon_{\alpha}}\right) \end{aligned}$$

$$\begin{aligned} \mathrm{valid\ for}_{riminite^{\alpha}\ gas} \\ &= \mu a \operatorname{abolic\ traps}_{lust\ the\ same} \end{aligned}$$

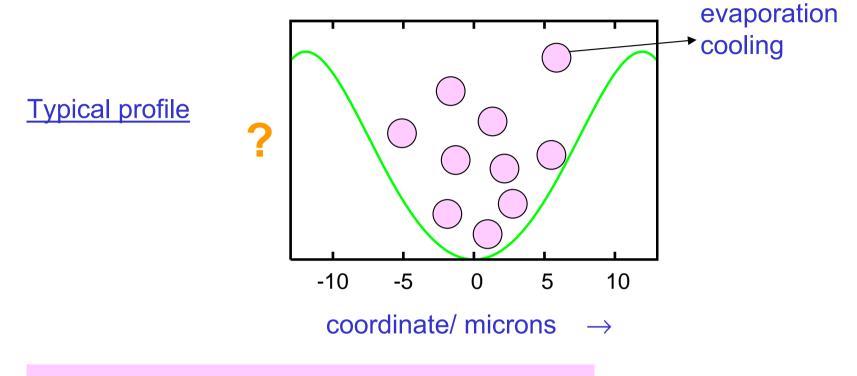
## Non-interacting bosons in a trap

## Useful digression: energy units

energy	1K	1eV	s <sup>-1</sup>
1K	$k_{ m B}/{ m J}$	$k_{\rm B}$ / $e$	$k_{ m B}$ / $h$
1eV	$e/k_{\rm B}$	e/J	e/h
s <sup>-1</sup>	$h/k_{\rm B}$	h/e	h/J

energy	1K	1eV	s <sup>-1</sup>
1K	$1.38 \times 10^{-23}$	$8.63 \times 10^{-05}$	$2.08 \times 10^{+10}$
1eV	$1.16 \times 10^{+04}$	$1.60 \times 10^{-19}$	$2.41 \times 10^{+14}$
s <sup>-1</sup>	$4.80 \times 10^{-11}$	$4.14 \times 10^{-15}$	$6.63 \times 10^{-34}$

## LAST TIME Trap potential



This is just one direction

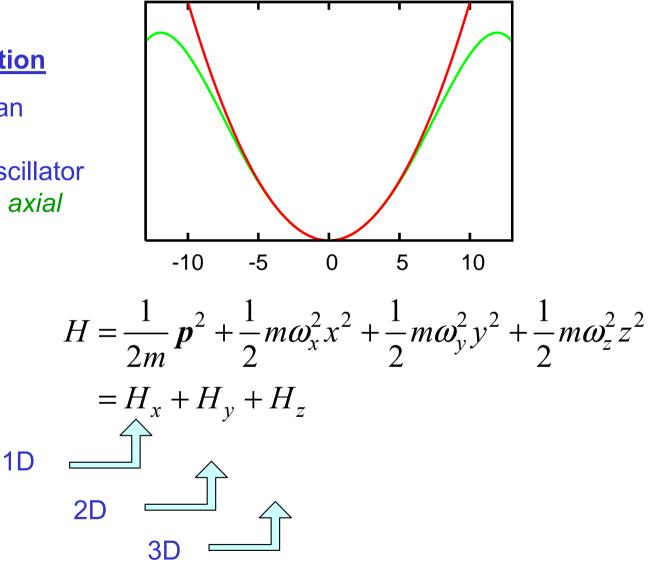
Presently, the traps are mostly 3D

The trap is clearly from the real world, the atomic cloud is visible almost by a naked eye

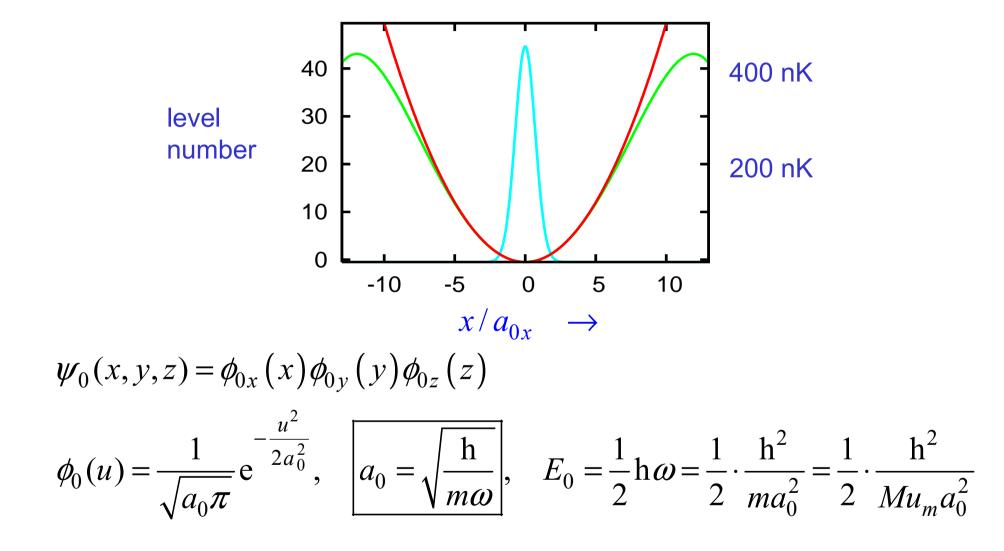
## LAST TIME Trap potential

#### Parabolic approximation

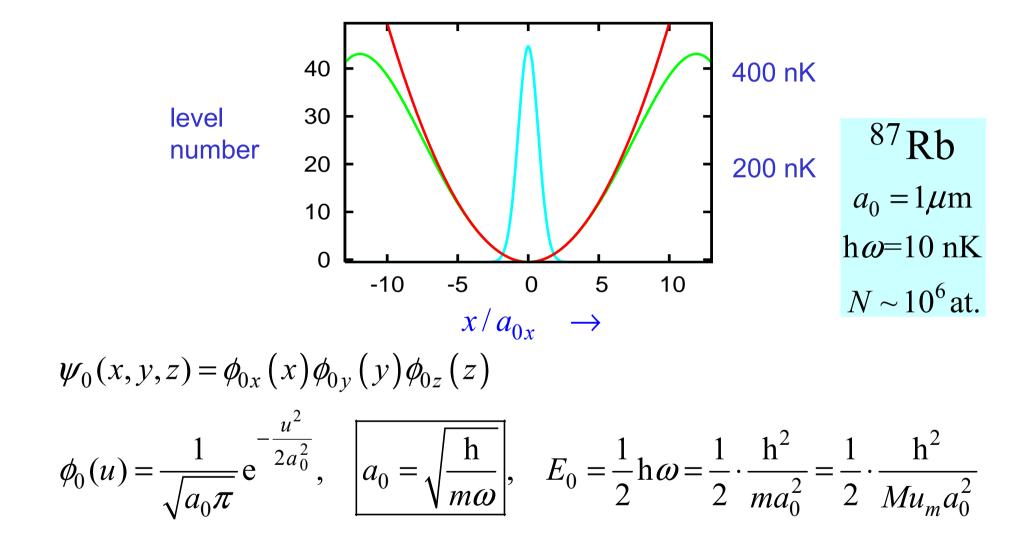
in general, an anisotropic harmonic oscillator usually with axial symmetry



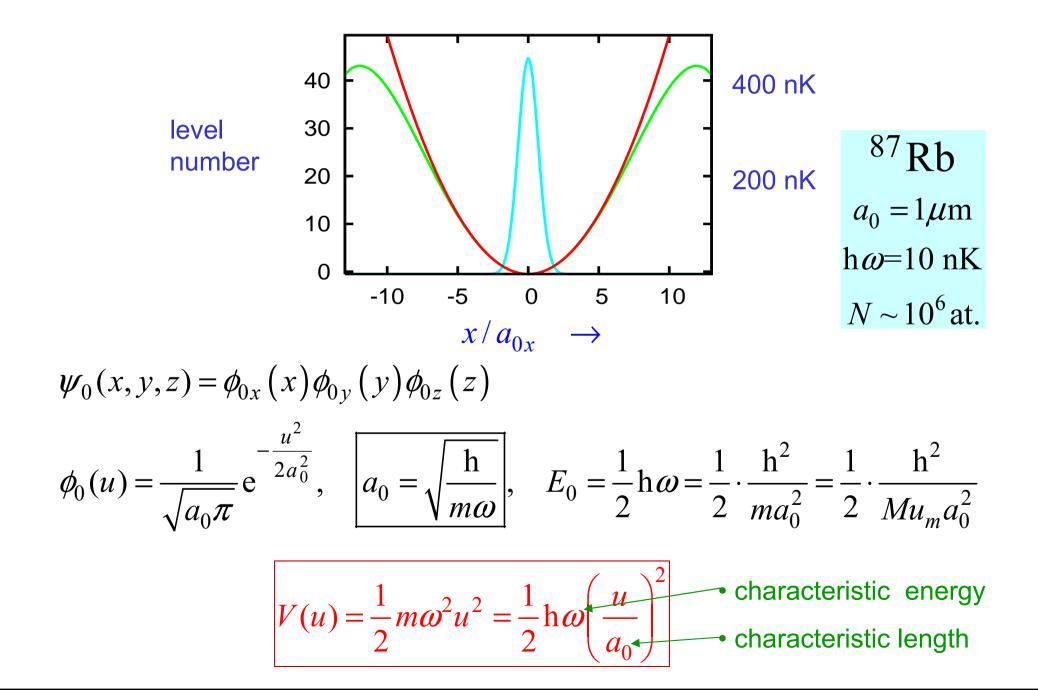
#### LAST TIME Ground state orbital and the trap potential



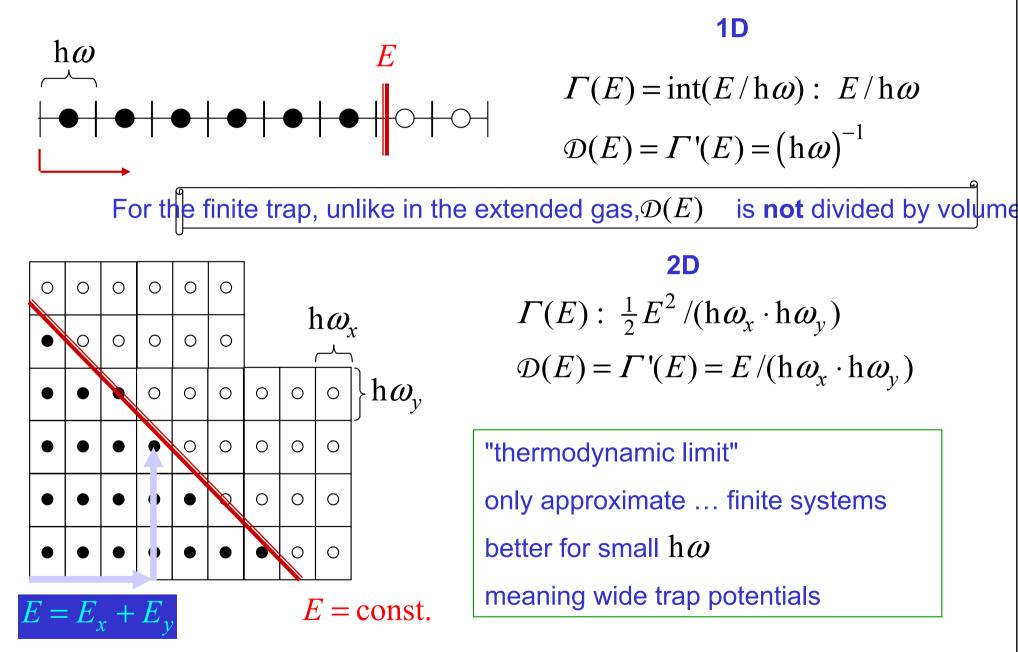
#### LAST TIME Ground state orbital and the trap potential



#### LAST TIME Ground state orbital and the trap potential



## Filling the trap with particles: IDOS, DOS



Filling the trap with particles

 $\mathbf{3D}$   $\Gamma(E): \frac{1}{6}E^3 / (\mathbf{h}\omega_x \cdot \mathbf{h}\omega_y \cdot \mathbf{h}\omega_z)$   $\mathcal{D}(E) = \Gamma'(E) = \frac{1}{2}E^2 / (\mathbf{h}\omega_x \cdot \mathbf{h}\omega_y \cdot \mathbf{h}\omega_z)$ 



particle number comparable with the number of states in the thermal shell

 $N \approx \Gamma \left( k_{\rm B} T \right)$ 

Filling the trap with particles

 $\mathbf{3D}$   $\Gamma(E): \frac{1}{6}E^3 / (\mathbf{h}\omega_x \cdot \mathbf{h}\omega_y \cdot \mathbf{h}\omega_z)$   $\mathcal{D}(E) = \Gamma'(E) = \frac{1}{2}E^2 / (\mathbf{h}\omega_x \cdot \mathbf{h}\omega_y \cdot \mathbf{h}\omega_z)$ 



particle number comparable with the number of states in the thermal shell

 $N \approx \Gamma \left( k_{\rm B} T \right)$ 

 $\begin{array}{lll} \hline 2 \mathbf{D} & T_c \approx \mathbf{h} \partial \phi \, k_{\mathrm{B}} \cdot N^{\frac{1}{2}} & \partial \phi = \left( \omega_x \cdot \omega_y \right)^{\frac{1}{2}} \\ \hline 3 \mathbf{D} & T_c \approx \mathbf{h} \partial \phi \, k_{\mathrm{B}} \cdot N^{\frac{1}{3}} & \partial \phi = \left( \omega_x \cdot \omega_y \cdot \omega_z \right)^{\frac{1}{3}} \\ \hline \mathbf{For 10^6 particles,} & \mathbf{o} \text{ characteristic energy} \\ & k_{\mathrm{B}} T_c \approx 10^2 \, \mathbf{h} \partial \phi & \mathrm{important for therm. limit} \end{array}$ 

#### Exact expressions for critical temperature etc.

The general expressions are the same like for the homogeneous gas. Working with discrete levels, we have

$$N = \mathcal{N}(T, \mu) = \sum_{j} \left\langle n(\varepsilon_{j}) \right\rangle = \sum_{j} \frac{1}{e^{\beta(\varepsilon_{j} - \mu)} - 1}$$

and this can be used for numerics without exceptions.

In the approximate thermodynamic limit, the old equation holds, only the volume V does not enter as a factor:

$$N = \mathcal{N}(T, \mu) = \frac{1}{e^{\beta(\varepsilon_0 - \mu)} - 1} + \mathcal{N} \int_0^\infty d\varepsilon \frac{1}{e^{\beta(\varepsilon - \mu)} - 1} \mathcal{D}(\varepsilon)$$
  
In 3D,  
$$T_c = (\zeta(3))^{-\frac{1}{3}} h \partial \partial \delta k_B \cdot N^{\frac{1}{3}} = 0.94h \partial \delta \delta k_B \cdot N^{\frac{1}{3}}$$
$$N_{BE} = N \cdot \left(1 - (T/T_c)^3\right), \quad T < T_c$$

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### How good is the thermodynamic limit

1D illustration (almost doable)

$$N = \sum_{j} \frac{1}{e^{\beta(h\omega \times j - \mu)} - 1} \stackrel{?}{=} \frac{1}{e^{-\beta\mu} - 1} + \int_{0}^{\infty} d\varepsilon \frac{1}{e^{\beta(\varepsilon - \mu)} - 1} \frac{1}{h\omega}$$

## How good is the thermodynamic limit

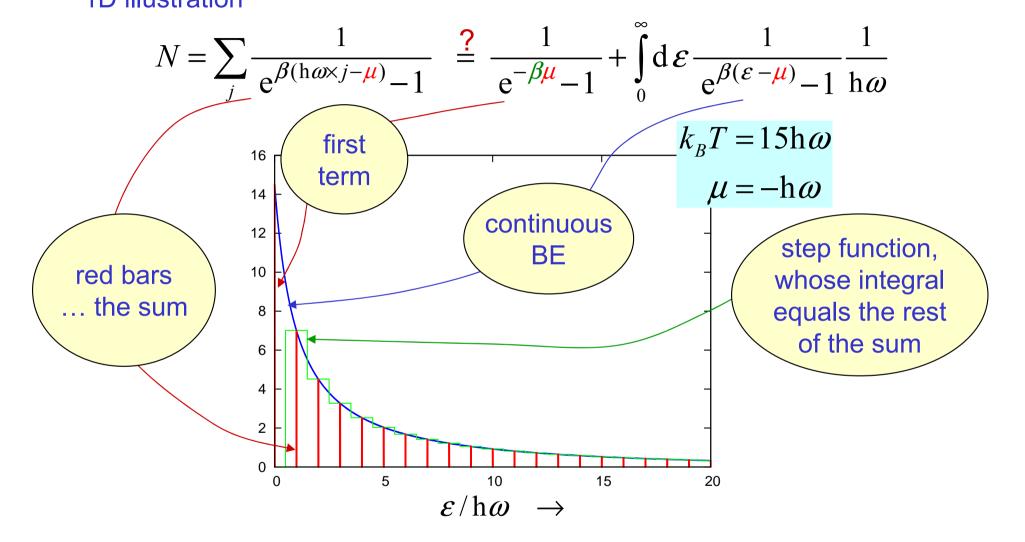
**1D illustration** 

$$N = \sum_{j} \frac{1}{e^{\beta(h\omega \times j - \mu)} - 1} \stackrel{?}{=} \frac{1}{e^{-\beta\mu} - 1} + \int_{0}^{\infty} d\varepsilon \frac{1}{e^{\beta(\varepsilon - \mu)} - 1} \frac{1}{h\omega}$$

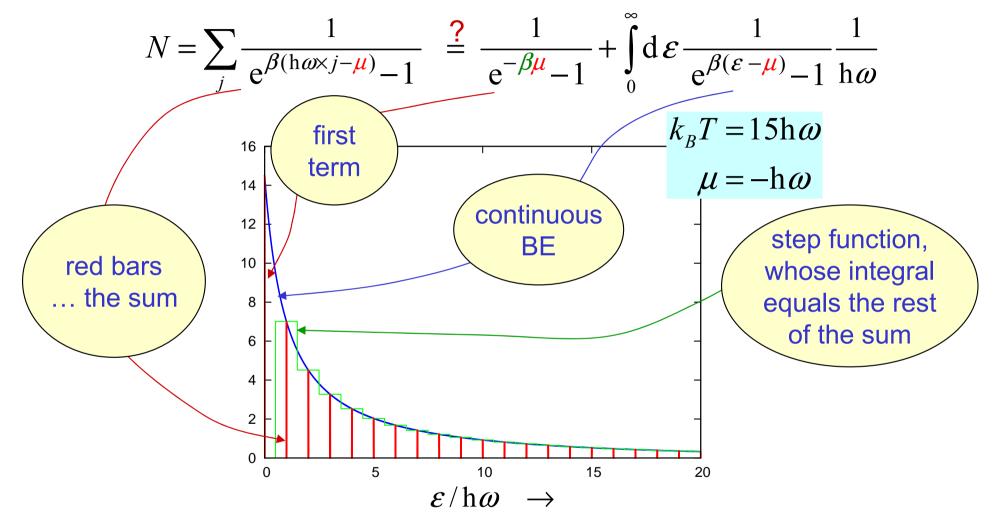
$$k_{B}T = 15h\omega$$

$$\mu = -h\omega$$

# How good is the thermodynamic limit 1D illustration



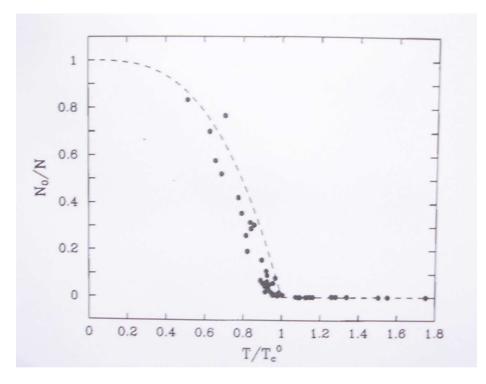
# How good is the thermodynamic limit 1D illustration



The quantitative criterion for the thermodynamic limit

$$\frac{k_{\scriptscriptstyle B}T_{\scriptscriptstyle C}}{\mathrm{h}\omega}?$$

## How sharp is the transition



These are experimental data fitted by the formula  $N_{\rm BE} = N \cdot (1 - (T/T_c)^3), \quad T < T_c$ 

The rounding is apparent, but not really an essential feature

## The end